EXPGUI: Smoothing the Path to Powder Crystallography

Back in the dark ages of computational crystallography, crystallographers were expected to be able to modify their computer programs to suit the computation at hand. Most crystallographers could create programs to convert data between different formats, and felt comfortable reading through a program's source code when the program documentation did not adequately explain a topic. (There is disagreement on when this ended, some say the 1950s, others say the 1980s or even the early 21st century!)

The advent of desktop computing has also introduced a new paradigm of computing — the graphical user interface (GUI). Visual analogies to physical devices (such as switches) make operating a GUI intuitive; a good GUI implementation significantly reduces learning time.

Simultaneous with the changes in computing, crystallography has evolved from a technique used exclusively by specialists to one of many tools in the arsenal of chemists, physicists and engineers. To facilitate this, the NCNR is developing GUI-based software for crystallography. There are two goals: to increase the utility of the software for the non-specialist, and to improve the productivity of experts. This allows novices to concentrate on the science and techniques of neutron powder crystallography rather than devote their efforts to learning arcane details of computer software.

The Rietveld refinement technique for crystallographic analysis was adopted within the NCNR immediately after its first publication [1]. The NCNR then produced Rietveld software specifically adapted to the local instrumentation, which is still being improved [2, 3]. However, the General Structure Analysis System (GSAS) package of programs from Los Alamos is also widely used [4]. GSAS has wide applicability. It can be used with virtually any type of neutron or x-ray diffraction data, including both powder and single crystal data. It supports a wide range of geometric and compositional restraints and constraints. While many new features have been added to GSAS on a continual basis, the original text-based user interface has not changed. Novice and occasional users often find the many levels of dialogs cumbersome and difficult to learn.

Work on a GUI for GSAS was begun several years ago, with the modest goal of providing a mechanism for accessing a small portion of the GSAS features. The project, now called EXPGUI, has grown in scope [5]. Most of the commonly used powder diffraction features are now implemented, allowing a complete Rietveld refinement to be performed graphically. Features not implemented in the GUI can still be accessed via the standard GSAS user interface. EXPGUI runs identically on all platforms where GSAS is supported, including both Unix and Windows. In FY2001, the Advanced Technology Program recognized the value of this effort and provided funding to accelerate development.

The GUI is designed to display information and controls in a concise and intuitive fashion. An example screen, shown in Fig. 1, manipulates structural parameters. This figure demonstrates how four atoms that share sites in this material can be selected together, so that their refinement options can be changed as a group. Another screen, shown in Fig. 2, applies constraints that link appropriate parameters in the refinement.

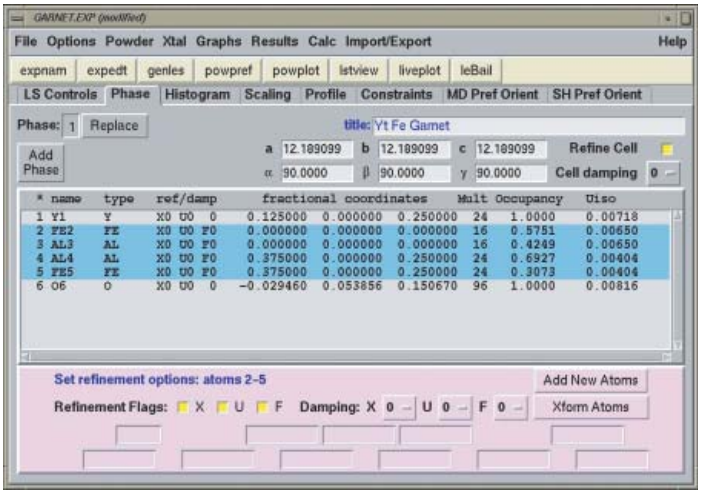

FIGURE 1. Sample screen from EXPGUI, showing where atomic parameters are displayed.

Recent EXPGUI development has been aimed at extending the capabilities of the GSAS package. As an example, when EXPGUI was recently given the ability to import atomic coordinates from files, support was added for CIF, the complex standard crystallographic information file format developed by the International Union of Crystallographers. Further, the import routine was written in a general fashion, so that other formats are easy to add.

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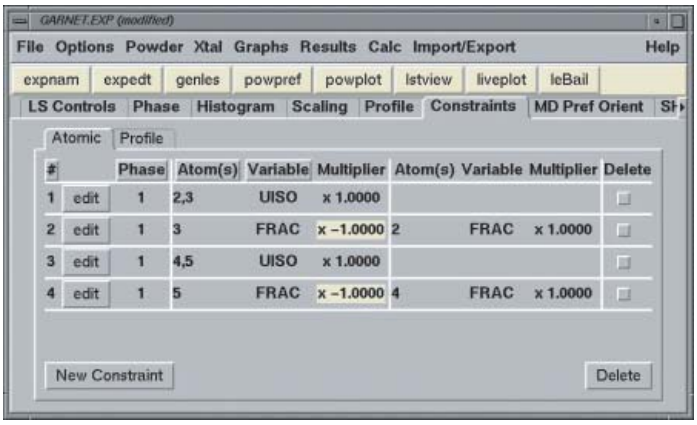

FIGURE 2. EXPGUI screen for entering and display of atomic constraints. In this case, atoms sharing sites are constrained to have the same U_{iso} values and have fractional occupancies that total to unity.

Where possible, EXPGUI takes advantage of the graphical nature of modern computers to offer scientists better access to refinement tools. Figure 3 shows a graphical display of the observed and computed diffraction pattern. Through a simple set of mouse operations, the user has "zoomed in" on a portion of the data, to better see the poor agreement between observed and computed intensity values, indicating that the structure is not well modeled.

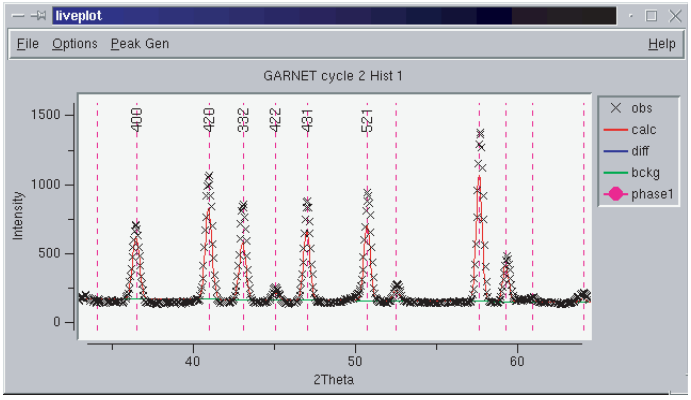

FIGURE 3. Graphical display of fit in EXPGUI. This plot has been "zoomed" in to show details. Several features of this plot, for example the display of reflection indices and the location of the fitted background, were not previously available in GSAS.

This graphical tool also allows the user to see the fitted background and to label the reflection indices — features not previously available within GSAS. Another example is a new tool for background fitting. In most cases, background fitting is nearly automatic, but for some refinements, fitting can be quite difficult. GSAS allows a scientist to define the background either through use of a function with refinable terms or as a spline drawn through a set of fixed points. A new tool in EXPGUI improves GSAS by allowing a user to define where the background curve should occur using a computer mouse. Since many experts agree that fixed background points are a poor way to treat background fitting, EXPGUI offers an augmented feature: a background function can be fit to the user's desired background curve. The terms for this function will be sufficient to obtain an initial model with good agreement to the data. At the end, the background terms can be optimized, to obtain the best possible model. This capability was not previously available in GSAS.

EXPGUI has been widely adopted by Rietveld users. It is used in most major neutron and synchrotron facilities, as well as dozens, if not hundreds, of universities, companies and research centers around the world.

References

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